Integrated Thermo-mechanical Design of of First Wall Components Under Evolving Chemistry and Microstructure During Fusion Reactor Operation

ThermChem-FW

(An FES/Scidac-5 Center)

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UCLA · Stony Brook University · MIAMI · SciDAC Scientific Discovery through Advanced Computing · INL Idaho National Laboratory · Oak Ridge National Laboratory · Pacific Northwest National Laboratory

Project senior personnel

Marian (Mat)

Trelewicz (Mat)

- Szlufarska (Mat)
- Morgan (Mat)

Po (Mat)

Cereceda (Mat)

- Permann (Math)
- Spencer (Math)

- Bernholdt (CS)
- Humrickhouse (Mat)

- Cusentino (Mat)
- Sargsyan (Math)

- Setyawan (Mat)

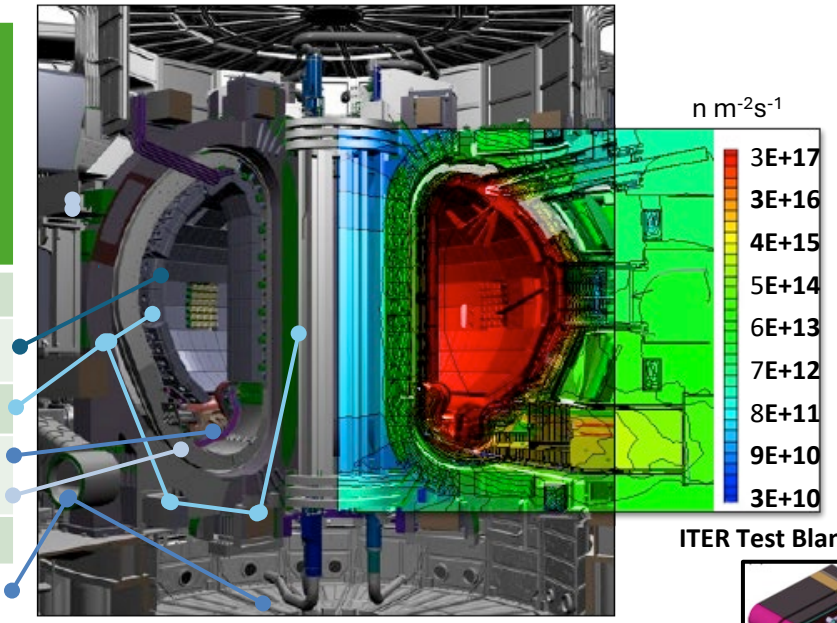
Plus :

- 6 Staff scientists (applied mathematicians, materials scientists, and computer scientists).
- 4 postdoctoral scholars
- 6 PhD students

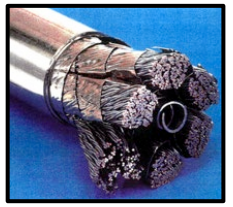
The significant gap bridging materials from ITER to Fusion Power Plant

Virtually no materials systems currently used are reactor viable

ITER Lifetime Neutron Fluence ($n\ cm^{-2}$)	Fusion Power Reactor Annual Neutron Fluence ($n\ cm^{-2}$)	
3.7E+21	5E+22	Blanket
5.1E+14	7E+15	Magnet
1.9E+21	2.6E+22	Divertor
1.1E+19	1.5E+20	Vacuum Vessel
3.4E+11	4.5E+12	Cryostat

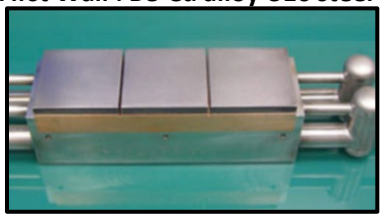


Magnet



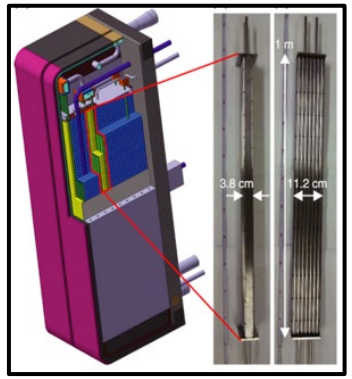
Diagnostic

First Wall : Be-Cu alloy-316 steel



Divertor: W-Cu alloy-316 steel

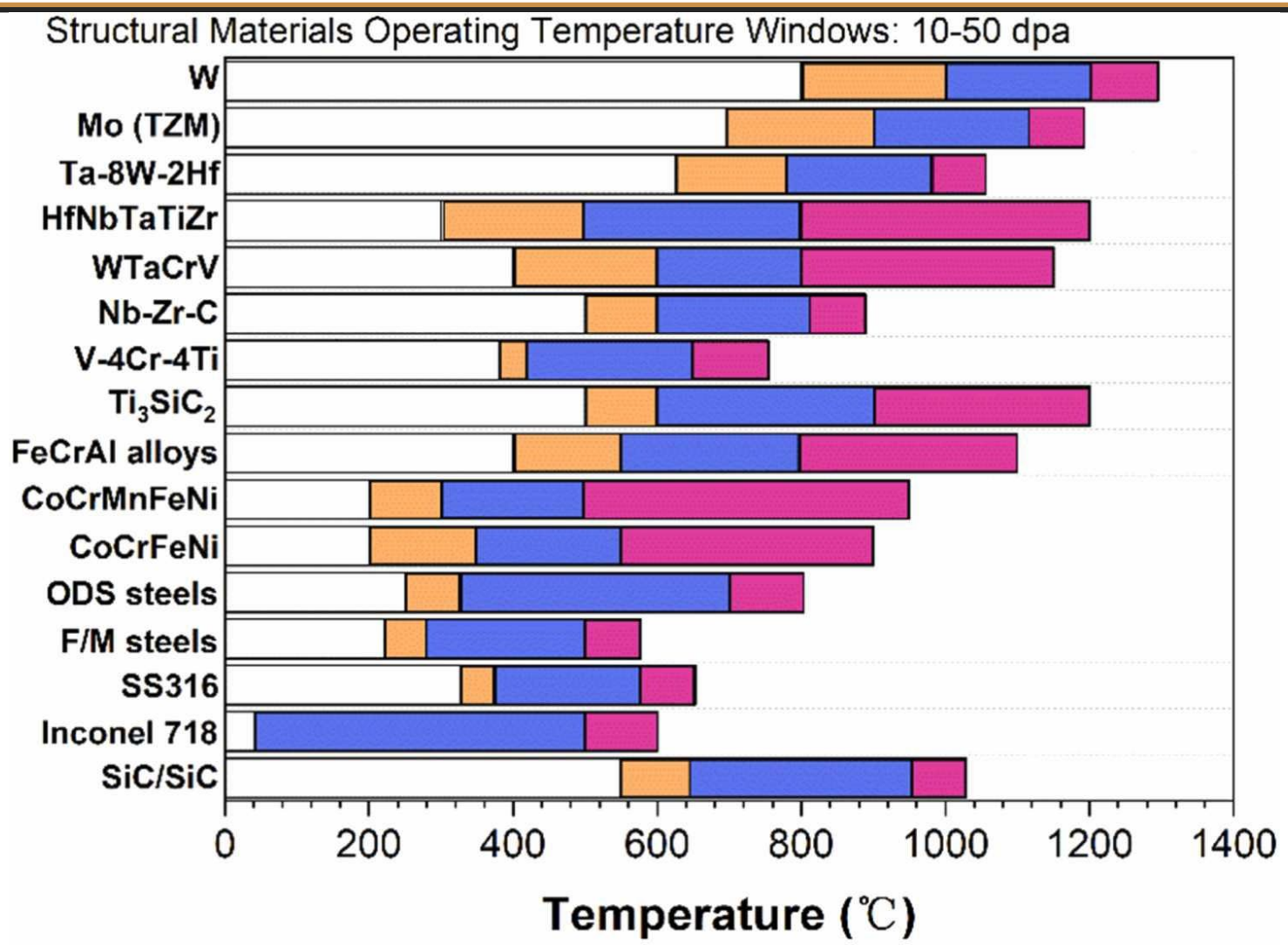
ITER Test Blanket Module: RAF Steel



Lack of fusion neutron source for materials testing!

Theory, modeling and simulation poised to play a key role in advancing our understanding of materials under fusion conditions

Temperature windows for fusion structural materials



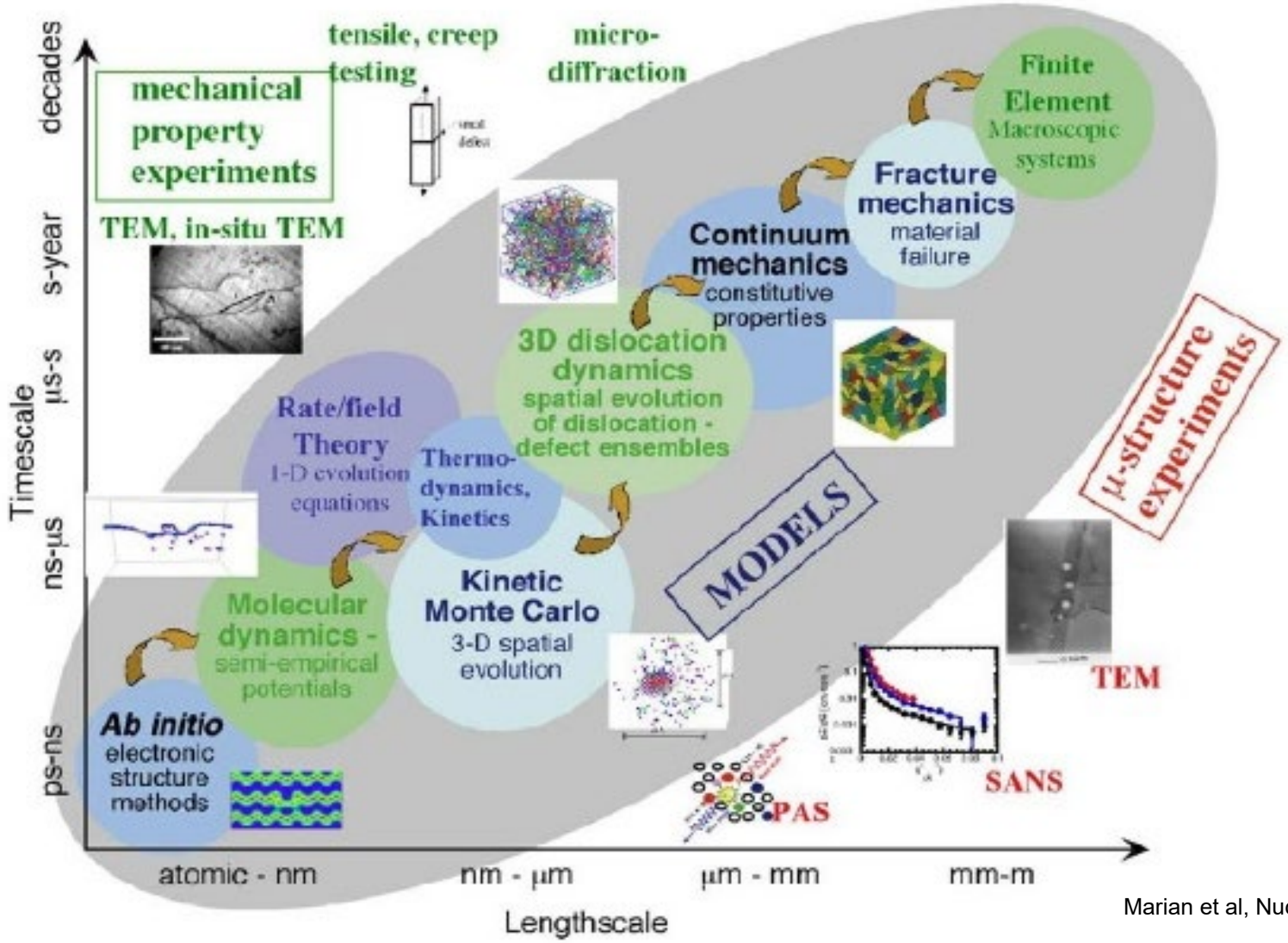
Uncertainties associated with: Irradiation hardening, Irradiation creep, swelling

Safe temperature window

Uncertainties associated with: Thermal creep, He embrittlement, thermal softening

Cheng, Zhaoyi, et al. "Irradiation effects in high-entropy alloys and their applications." *Journal of Alloys and Compounds* 930 (2023): 166768.

The multiscale modeling paradigm in irradiation damage



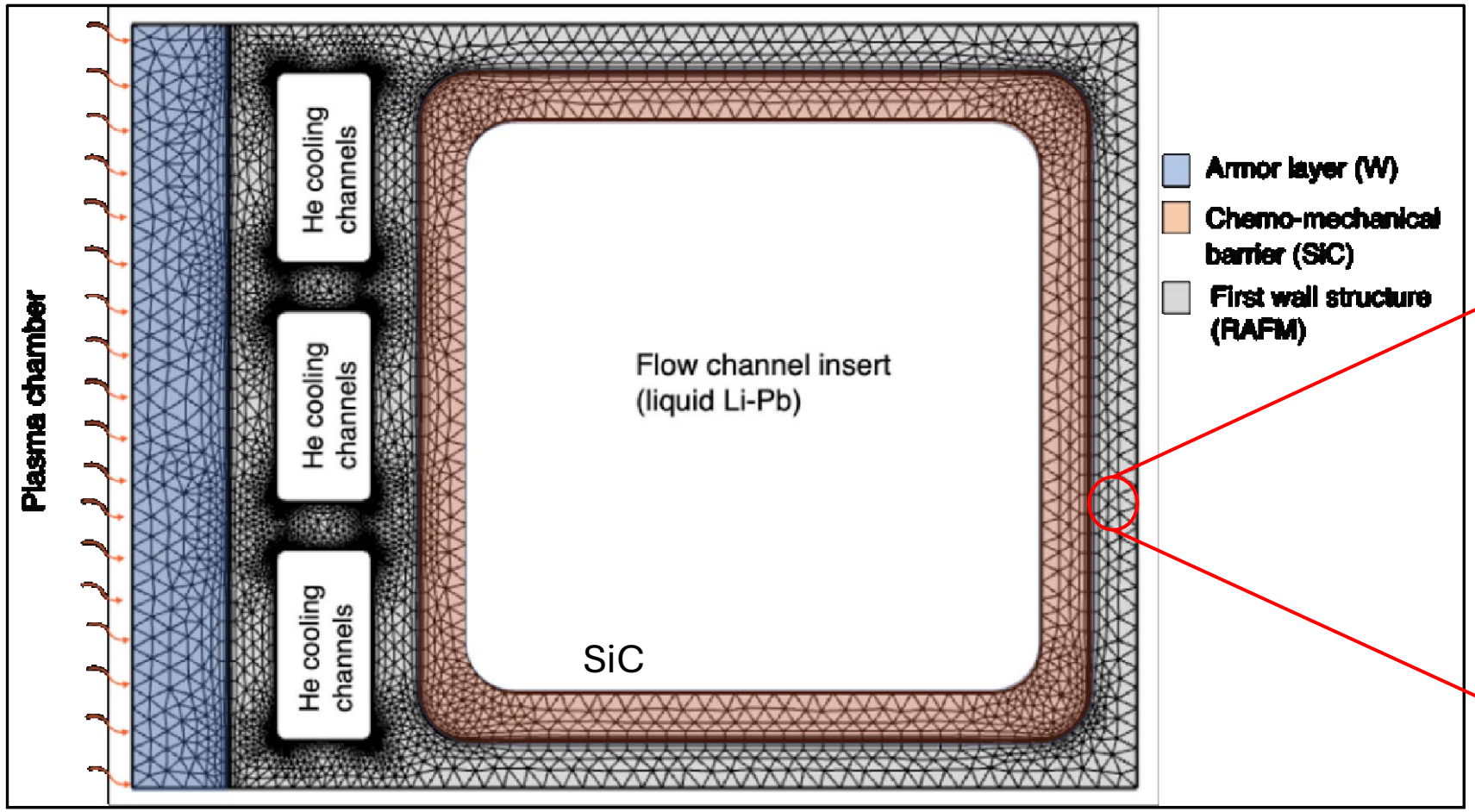
Marian et al, Nuclear Fusion (2015)

ThermChem-FW Center

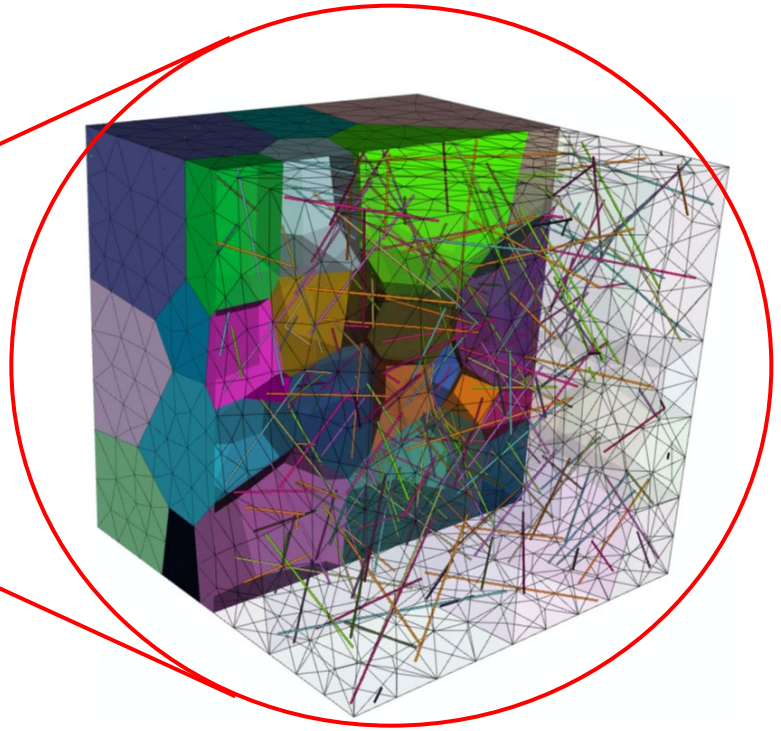
Capturing the effect of atomic-level processes due to neutron irradiation on fusion structural materials a components represents an unsolved ***computational grand challenge*** requiring of multidisciplinary teams with complementary expertise.

Materials scientistis, applied mathematicians, and computer scientists working together to develop models, algorithms, and software to solve some of the most pressing issues for fusion structural materials.

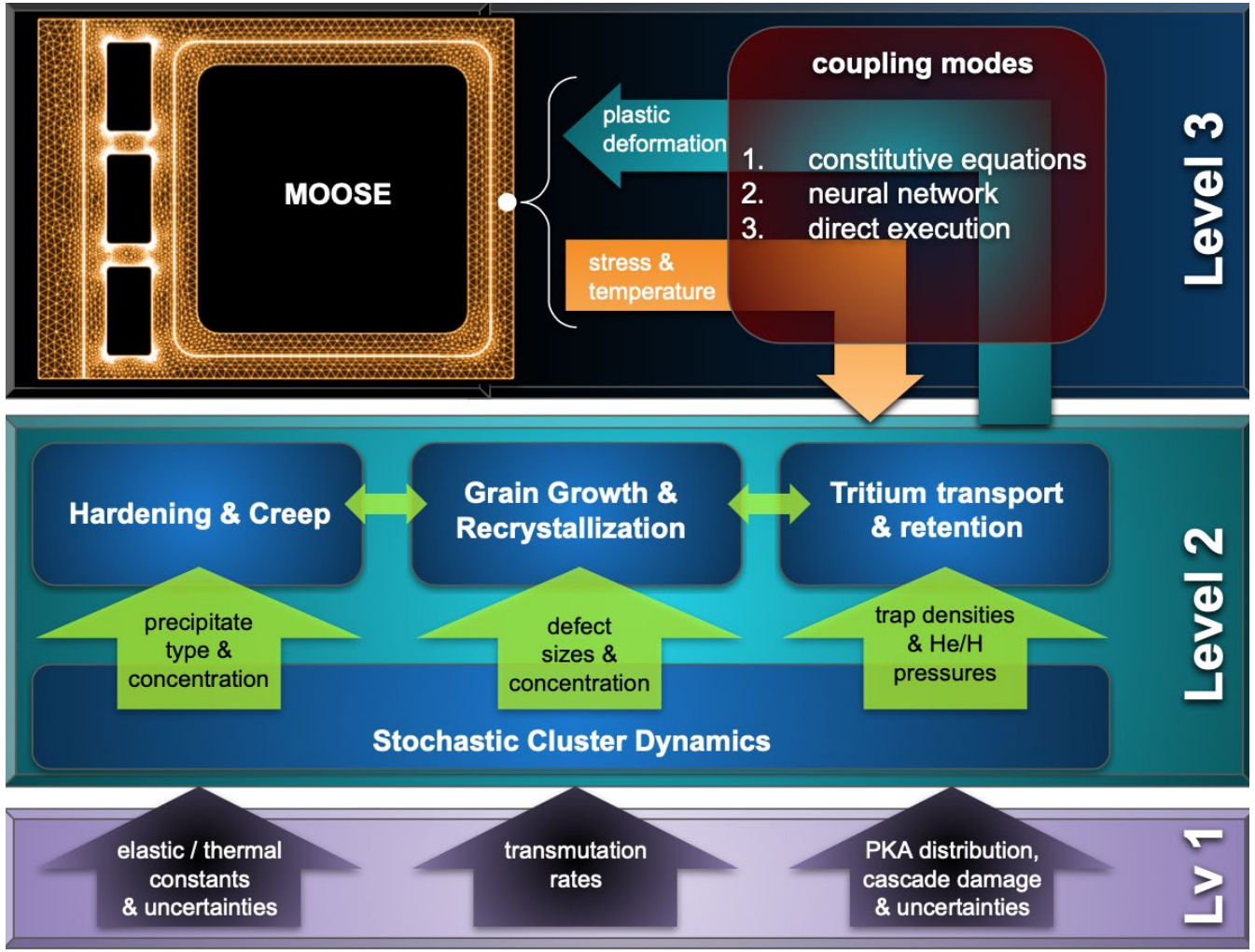
Reference fusion first wall module used as testbed for models



Physics based model with full spatio-temporal resolution



The project has been structured as a connected multi-level workflow

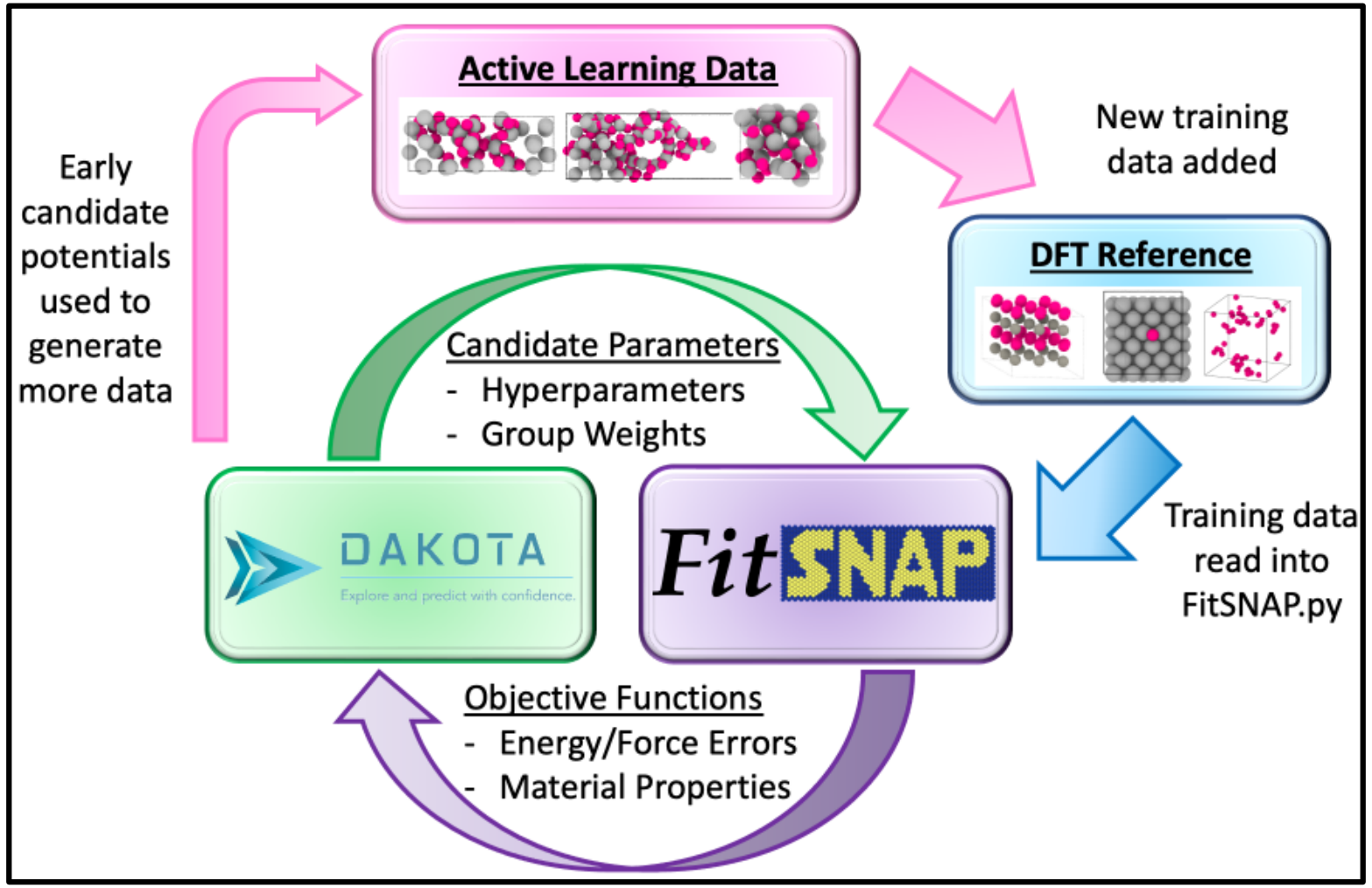


Level 3 involves time-dependent simulations (using the finite element code MOOSE) of the thermomechanical evolution of the full FW/B structure. These models will capture the entire geometric complexity and diversity of the multi-material FW/B and will furnish component lifetime prediction and design recommendations based on stress distributions and material property degradation.
INL, ORNL, Miami

Level 2 operates at mesoscopic scales where microstructural evolution occurs, including irradiation hardening, irradiation creep and swelling, thermal fatigue, precipitation, recrystallization (grain growth), and tritium permeation and retention.
UCLA, Miami, ORNL

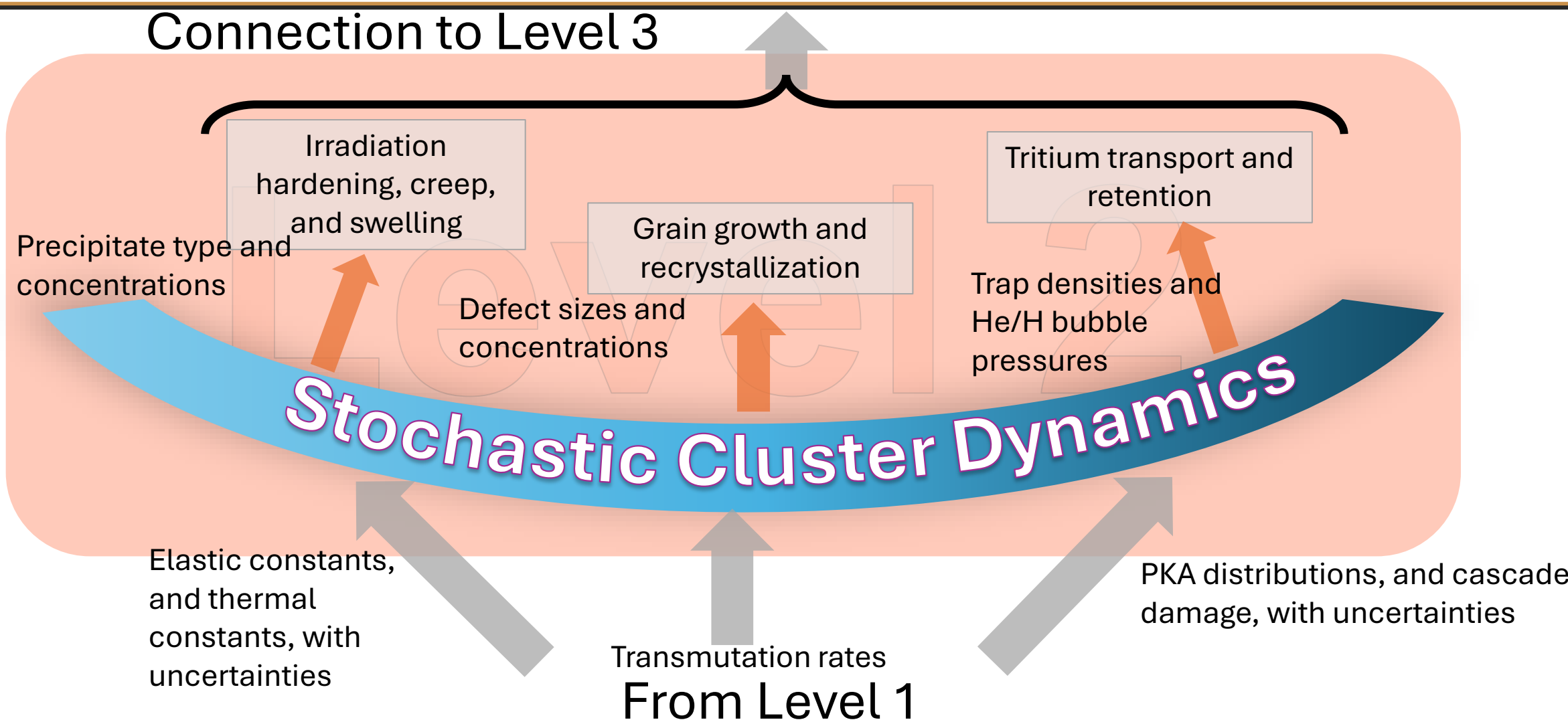
Level 1 captures atomic-level physical processes representative of fusion reactor operation in the FW/B structure, such as (i) transmutation, primary knock-on atoms (PKA) distributions, (ii) cascade damage, (iii) interactions of defect clusters, and (iv) tritium uptake, trapping, and diffusion.
Stony Brook, Wisconsin, Villanova, SNL

Level 1: Atomistics (ps~ns, ~nm)

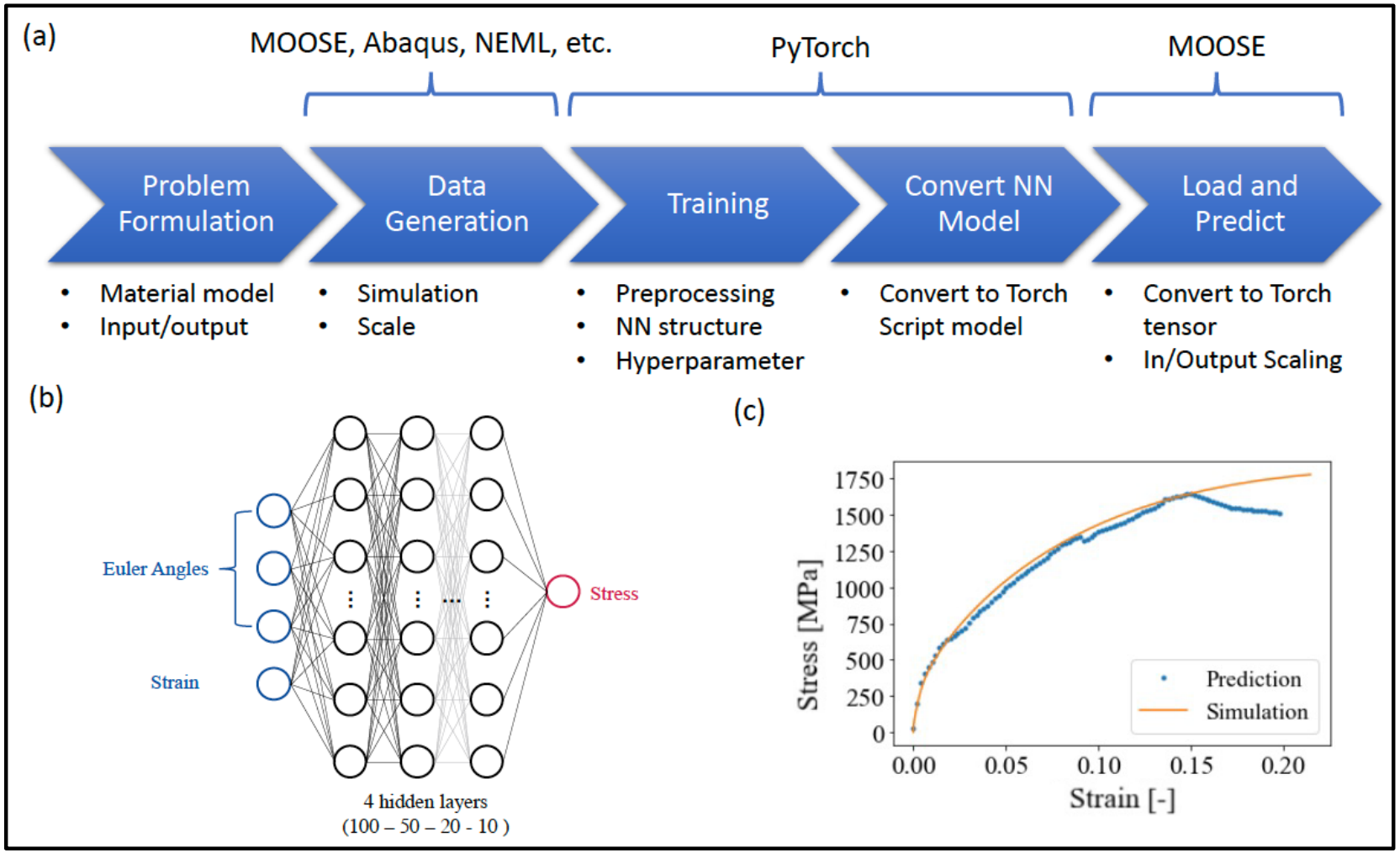


- Atomistic simulations are intended to provide fundamental material property changes under a set of conditions that mimics operational scenarios.
- Data-based machine-learned interatomic potentials are being developed for structural materials consisting of complex chemical isotope inventories caused by nuclear transmutation.
- These potentials will be employed in molecular dynamics simulations of physical property changes in the corresponding materials.
- Uncertainties are built into these potentials using NN-based ML-interatomic potentials.

Level 2: Microstructure (~ms, microns)



Level 3: Continuum (~s, ~cm)

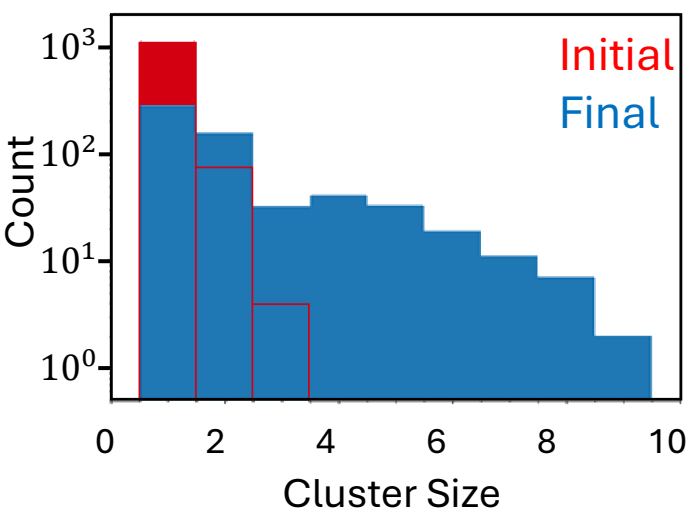


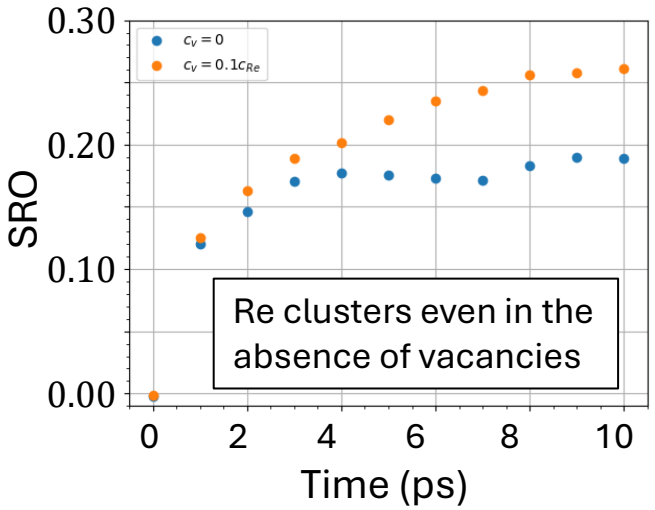
Level 2 simulations will be the basis for 'reduced order models' (ROM) that will be coupled to the multipurpose finite element code MOOSE.

The figure to the left shows a diagram with the integration of a set of ROM into the code.

Progress on MD Simulations in W-Re

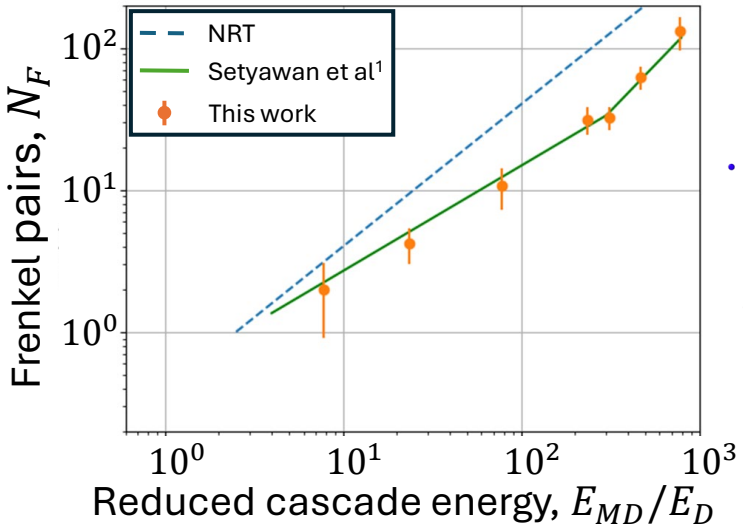
Transmutant segregation via combined Monte Carlo and Molecular Dynamics

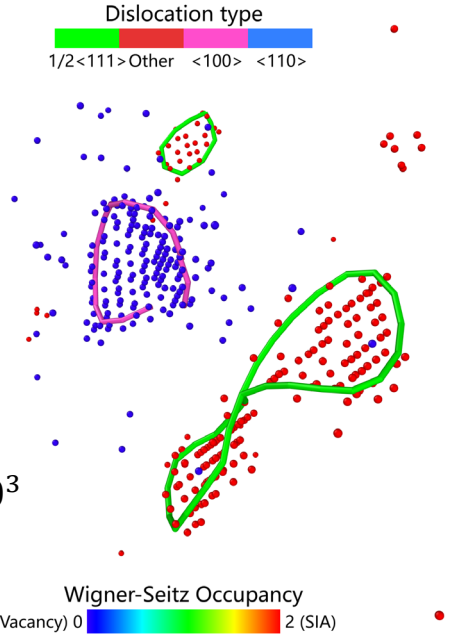




Re clustering without vacancies due to erroneous Re-Re binding energy in EAM potential highlights motivation for SNAP potential

Displacement Cascades via Molecular Dynamics

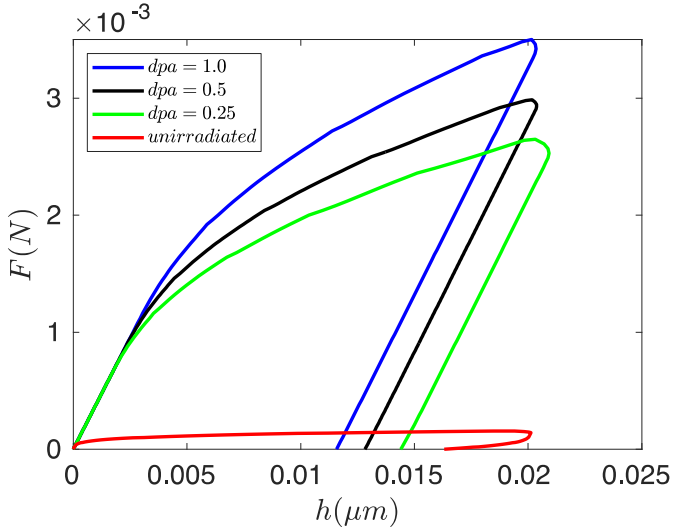


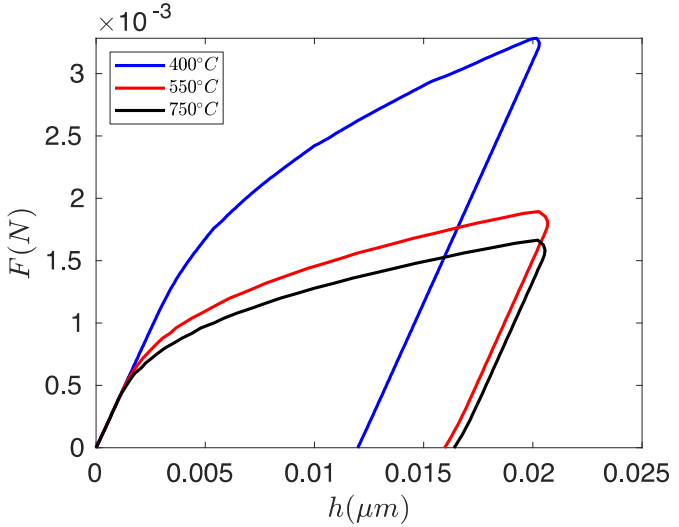


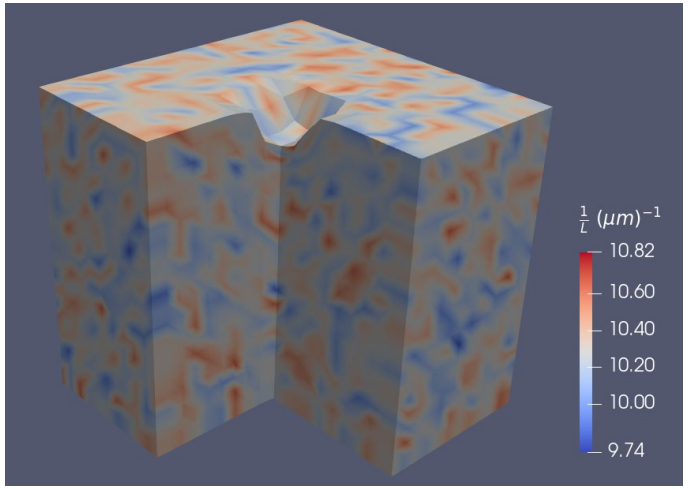
Measuring point defect and dislocation loop generation in pure W displacement cascades

[1]Setyawan, W., et al. (2015). Displacement cascades and defects annealing in tungsten, Part I: Defect database from molecular dynamics simulations. *Journal of Nuclear Materials*, *462*, 329-337.

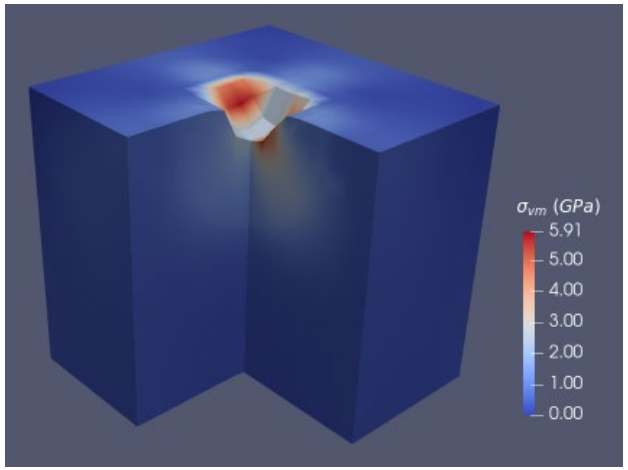
Nanoidentation simulations in irradiated W







(a)



(b)

Collaboration resources

- The project mailing list (thermchem-fw@email.ornl.gov)
- The Box workspace we use for internal file sharing (https://ucla.box.com/s/o2unb7df1ep12g1lefdwsm7e0fmttf49)
- The Slack workspace we use for informal communications (https://thermchem-fwscidac.slack.com/home)
- The GitHub team(s) associated with our GitHub organization (https://github.com/ThermChem-FW)

- Our website: https://thermchem-fw.github.io/
  - Which uses the Jekyll static site generation tool and is hosted in this repository: https://github.com/ThermChem-FW/thermchem-fw.github.io
- Information on accessing various computing facilities here: Computer Access.boxnote